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Temporal convergence analysis of a locally implicit discontinuous Galerkin time domain method for electromagnetic wave propagation in dispersive media

Stéphane Descombes^{a,*}, Stéphane Lanteri^b, Ludovic Moya^b

^a*Université Côte d'Azur, CNRS, Inria, LJAD, France,*

^b*Université Côte d'Azur, Inria, CNRS, LJAD, France*

Abstract

This paper is concerned with the approximation of the time domain Maxwell equations in a dispersive propagation medium by a Discontinuous Galerkin Time Domain (DGTD) method. The Debye model is used to describe the dispersive behaviour of the medium. We adapt the locally implicit time integration method from [1] and derive a convergence analysis to prove that the locally implicit DGTD method for Maxwell-Debye equations retains its second order convergence.

Keywords: Maxwell's equations, time domain, dispersive medium, discontinuous Galerkin method, convergence analysis

1. Introduction

We consider the propagation of electromagnetic waves in dispersive media. These are materials in which either or both of the electromagnetic material parameters ε , the electric permittivity, and μ , the magnetic permittivity are functions of frequency. We will focus on the much more common case of frequency-dependent permittivity. A lot of practical problems involve such propagation media, such as modeling the interaction of an electromagnetic wave with biological tissues. The numerical modeling of the propagation

*Corresponding author.

Email addresses: `stephane.descombes@unice.fr` (Stéphane Descombes), `stephane.lanteri@inria.fr` (Stéphane Lanteri), `ludovic.moya@inria.fr` (Ludovic Moya)

of electromagnetic waves through human tissues is at the heart of many biomedical applications such as the microwave imaging of cancer tumours. Accurate and efficient numerical modeling techniques, are required to deal with the complex issues characterizing the associated propagation problems.

Numerical simulation of wave propagation in dispersive media started in early 1990's in the framework of Finite Difference Time Domain (FDTD) methods, for details and references see e.g. [2] chapter 2 or [3] chapter 3. Finite Elements Time Domain (FETD) methods were not explored until 2001 [4] and DGTD methods for solving Maxwell's equations in dispersive media have been considered more recently. In [5, 6], a priori error estimates are proved for the second order formulation of Maxwell's equations coupled to dispersive models discretized by an interior penalty DG formulation. Some two-dimensional numerical tests are included for supporting the provided analysis. In [7], different dispersive media are treated, considering a locally divergence-free DG method. The scheme is written and studied in its semi-discretized version, while the fully discrete scheme is described but not analyzed. Finally, in [8], which deals with the Debye model, a centered flux discontinuous Galerkin formulation for the discretization in space is coupled with a second order leap-frog scheme for time integration. Stability estimates are derived through energy conservation and convergence is proved for both the semi-discrete and the fully discrete scheme. A two-dimensional artificial numerical problem is presented to validate the theoretical findings.

In this paper we still deal with the Debye model but in the presence of a locally refined mesh. In Section 2 we present the formulation of Maxwell's equations for Debye dispersive media. The Debye model is most often used to model electromagnetic wave interactions with water-based substances, such as biological materials. In Section 3 Maxwell's equations in dispersive media are discretized according to a centered flux DG formulation and due to the presence of a locally refined mesh we adapt the locally implicit time integration method from [1] and give a rigorous stability criterion. In Section 4 we derive a convergence analysis to prove that the locally implicit DGTD method retains its second order convergence. Finally, in Section 5, we present some numerical results concerning three-dimensional microwave propagation in biological tissues.

2. The continous problem

Let $\Omega \subset \mathbb{R}^3$ be a bounded, convex polyhedral domain, we denote by \vec{n} the normal outward to $\partial\Omega$. We consider the time domain formulation of Maxwell's equations in Ω used to model the propagation of an electromagnetic wave in a dispersive medium. In this dispersive medium, the effect of the electric field \vec{E} is described by the electric displacement \vec{D} with the formula

$$\vec{D} = \varepsilon_0 \varepsilon_\infty \vec{E} + \vec{P}, \quad (1)$$

ε_0 and ε_∞ being respectively the electric permittivity in vacuum and the infinite frequency relative permittivity, \vec{P} is the electric polarization. We assume that the medium is a single-pole Debye type dispersive medium implying that \vec{P} satisfies an ordinary differential equation of the form

$$\vec{P} + \tau \frac{\partial \vec{P}}{\partial t} = \varepsilon_0 (\varepsilon_s - \varepsilon_\infty) \vec{E}, \quad (2)$$

with ε_s , called the static relative permittivity i.e. the permittivity at zero frequency ($\varepsilon_s > \varepsilon_\infty$) and τ the Debye relaxation time constant, both of them being characteristic of the material. We can now state Maxwell's equations in a Debye dispersive medium. Let $T > 0$, the magnetic field \vec{H} , the electric field \vec{E} and the electric polarization \vec{P} satisfy after normalization in space and time (see [9]) the following system of equations for time $t \in [0, T]$

$$\begin{cases} \mu \frac{\partial \vec{H}}{\partial t} = -\text{curl}(\vec{E}), \\ \varepsilon_\infty \frac{\partial \vec{E}}{\partial t} = \text{curl}(\vec{H}) - \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} \vec{E} - \sigma \vec{E} + \frac{1}{\tau} \vec{P}, \\ \frac{\partial \vec{P}}{\partial t} = \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} \vec{E} - \frac{1}{\tau} \vec{P}, \end{cases} \quad (3)$$

μ and σ denoting respectively the relative magnetic permeability and the conductivity. Concerning the boundary conditions we impose on $\partial\Omega$ a metallic boundary conditions i.e. $\vec{n} \times \vec{E} = 0$ or a Silver-Müller condition, which is a first order approximation of the expansion in pseudo-differential operators of the exact radiation condition, given by

$$\vec{n} \times \vec{E} - \sqrt{\frac{\mu}{\varepsilon}} \vec{n} \times (\vec{H} \times \vec{n}) = \vec{n} \times \vec{E}^{inc} - \sqrt{\frac{\mu}{\varepsilon}} \vec{n} \times (\vec{H}^{inc} \times \vec{n})$$

where $(\vec{E}^{inc}, \vec{H}^{inc})$ is a given incident field. The purpose of this paper is to prove a second order convergence of a numerical scheme, we then assume (at least formally) that the solution is regular to perform and justify all the computations.

3. Locally implicit DGTD method

DG methods share almost all the advantages of FE methods (large spectrum of applications, complex geometries, etc.) and FV methods (ability to capture discontinuous solutions). The DG method has other nice properties which explain the renewed interest it gains in various domains in scientific computing as witnessed by books or special issues of journals dedicated to this method [10, 11, 12, 13]. Following the DG method discribed in [14], based on a centered numerical flux for the approximation of the boundary integral term at the interface between neighboring elements, we write the semi-discrete system as follows

$$\begin{cases} \mu M \frac{\partial H}{\partial t} = -S^T E, \\ \varepsilon_\infty M \frac{\partial E}{\partial t} = SH - \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} ME - \sigma ME + \frac{1}{\tau} MP, \\ M \frac{\partial P}{\partial t} = \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} ME - \frac{1}{\tau} MP, \end{cases} \quad (4)$$

H , E , P being column vectors and M and S the mass and flux matrices. Let us mention that other space discretizations, such as finite differences or vector finite elements, can also lead to semi-discrete system of the same form. Using the Cholesky factorization of the mass matrix $M = L_M L_M^T$, where L_M is a triangular matrix, introducing the new variables $L_M^T E$, $L_M^T H$ and $L_M^T P$ still denoted by H , E , P and the new matrix $L_M^{-1} S (L_M^{-1})^T$ still denoted by S , we rewrite (4) in the form

$$\begin{cases} \mu \frac{\partial H}{\partial t} = -S^T E, \\ \varepsilon_\infty \frac{\partial E}{\partial t} = SH - \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} E - \sigma E + \frac{1}{\tau} P, \\ \frac{\partial P}{\partial t} = \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} E - \frac{1}{\tau} P. \end{cases} \quad (5)$$

A simple time integration method that we can use to discretize the semi-discrete system (5) is the explicit second order leap-frog scheme given by

$$\left\{ \begin{array}{lcl} \mu \frac{H^{n+1/2} - H^n}{\Delta t/2} & = & -S^T E^n, \\ \varepsilon_\infty \frac{E^{n+1} - E^n}{\Delta t} & = & SH^{n+1/2} - \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E^{n+1} + E^n) \\ & & - \frac{1}{2}\sigma (E^{n+1} + E^n) + \frac{1}{2\tau} (P^{n+1} + P^n), \\ \frac{P^{n+1} - P^n}{\Delta t} & = & \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E^{n+1} + E^n) - \frac{1}{2\tau} (P^{n+1} + P^n), \\ \mu \frac{H^{n+1} - H^{n+1/2}}{\Delta t/2} & = & -S^T E^{n+1}. \end{array} \right.$$

Unfortunately in the presence of a locally refined mesh this explicit time integration method can lead to a severe time step size restriction. An implicit time integration scheme is a natural way to overcome this situation and we can apply the second order Crank-Nicolson scheme to the semi-discrete system (5) that we write in the three stage form

$$\left\{ \begin{array}{lcl} \mu \frac{H^{n+1/2} - H^n}{\Delta t/2} & = & -S^T E^n, \\ \varepsilon_\infty \frac{E^{n+1} - E^n}{\Delta t} & = & \frac{1}{2}S (H^{n+1} + H^n) - \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E^{n+1} + E^n) \\ & & - \frac{1}{2}\sigma (E^{n+1} + E^n) + \frac{1}{2\tau} (P^{n+1} + P^n), \\ \frac{P^{n+1} - P^n}{\Delta t} & = & \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E^{n+1} + E^n) - \frac{1}{2\tau} (P^{n+1} + P^n), \\ \mu \frac{H^{n+1} - H^{n+1/2}}{\Delta t/2} & = & -S^T E^{n+1}. \end{array} \right.$$

The solution of a global linear system at each time step obliterates one of the attractive features of discontinuous Galerkin formulations and an implicit-explicit time integration scheme can be viewed as a better solution. Extending the implicit-explicit method developed in [1] we blend the leap-frog scheme and the Crank-Nicolson scheme written in a three stage form to obtain the implicit-explicit time integration scheme for the semi-discrete

system (5)

$$\left\{ \begin{array}{l} \mu \frac{H^{n+1/2} - H^n}{\Delta t/2} = -S^T E^n, \\ \varepsilon_\infty \frac{E^{n+1} - E^n}{\Delta t} = S_0 H^{n+1/2} + \frac{1}{2} S_1 (H^{n+1} + H^n) \\ \quad - \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E^{n+1} + E^n) \\ \quad - \frac{1}{2} \sigma (E^{n+1} + E^n) + \frac{1}{2\tau} (P^{n+1} + P^n), \\ \frac{P^{n+1} - P^n}{\Delta t} = \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E^{n+1} + E^n) - \frac{1}{2\tau} (P^{n+1} + P^n), \\ \mu \frac{H^{n+1} - H^{n+1/2}}{\Delta t/2} = -S^T E^{n+1}, \end{array} \right. \quad (6)$$

where $S = S_0 + S_1$ is a matrix splitting. We adopt the splitting defined in [1], i.e. $S_1 = SS_H$, where S_H is the diagonal matrix of dimension the length of H defined by

$$(S_H)_{jj} = \begin{cases} 0, & \text{component } H_j \text{ of } H \text{ to be treated explicitly,} \\ 1, & \text{component } H_j \text{ of } H \text{ to be treated implicitly.} \end{cases}$$

A first question concerns the stability of the fully discrete locally implicit scheme (6). For this we define the discrete electromagnetic energy, denote \mathcal{E}_n , as

$$\mathcal{E}_n = \frac{1}{2} \left(\mu \|H^n\|_2^2 + \varepsilon_\infty \|E^n\|_2^2 + \frac{1}{(\varepsilon_s - \varepsilon_\infty)} \|P^n\|_2^2 - \frac{\Delta t^2}{4\mu} \langle S_0 S^T E^n, E^n \rangle \right), \quad (7)$$

where $\langle \cdot, \cdot \rangle$ is the L^2 inner product and $\|\cdot\|_2$ the corresponding norm. Defining by $\rho(S_0 S_0^T)$ the spectral radius of $S_0 S_0^T$, it is proven in [15], that under the assumption

$$\Delta t < \frac{2\sqrt{\varepsilon_\infty \mu}}{\sqrt{\rho(S_0 S_0^T)}},$$

the quadratic form \mathcal{E}_n is a positive definite quadratic form of the numerical unknowns H^n , E^n and P^n . Moreover \mathcal{E}_n is decreasing so that $\mathcal{E}_n \leq \mathcal{E}_0$ and this clearly yields the stability of the fully discrete locally implicit scheme (6).

4. Convergence analysis

In this section we are interested in the PDE convergence of the locally implicit method (6). We will examine whether the method retains its second order ODE convergence under stable simultaneous space-time grid refinement $\Delta t \sim h$, $h \rightarrow 0$ towards the exact PDE solution. This is not a priori clear due to the component splitting which can introduce order reduction through error constants which grow with h^{-1} , for $h \rightarrow 0$. An example of loss of order can be found in [16].

The derivations in the remainder of this section follow a method of lines analysis related to that of [1] for the locally implicit method which deals with Maxwell's equations but in non-dispersive media. The proof of second order temporal convergence in the PDE sense presented here is organized in three subsections. In Section 4.1 we will introduce the so-called perturbed scheme obtained by substituting the true PDE solution restricted to the assumed space grid into the locally implicit scheme (6). Herewith we introduce defects (truncation errors) composed of a temporal and a spatial error part. Our focus lies on temporal order, so for simplicity of derivation we will omit the spatial error part after this subsection. Indeed for our purpose, the spatial error part can be omitted without loss of generality. In Section 4.2 we derive the common temporal recurrence for the full global error which is the difference of the PDE solution restricted to the space grid and the numerical solution on this grid generated by scheme (6). Here we point out that this global error scheme needs to be transformed to overcome a spatial inconsistency in the local error emanating from component splitting. The crucial observation hereby is that this spatial inconsistency enters the temporal error by the negative power h^{-1} which kills one power of Δt as we assume $\Delta t \sim h$, $h \rightarrow 0$ (order reduction). Fortunately, this order reduction is present in the local error only and cancels in the transition from local to global errors. The fact that this cancellation occurs can be proved by transforming the global error scheme, which is shown in the third Section 4.3.

4.1. The perturbed scheme

Let $E_h(t)$ denote at time t the exact solution of the PDE problem restricted to the assumed space grid of the semi-discrete system (5), $E_h(t)$ is in fact the pointwise evaluation of the exact solution. $E_h(t_n)$ thus represents the vector that is approximated by E^n . Assume the same notation for H and P . Substituting $E_h(t)$, $H_h(t)$ and $P_h(t)$ into (5) reveals the spatial truncation

errors which we denote by ζ_h^E , ζ_h^H and ζ_h^P

$$\begin{cases} \mu \frac{d}{dt} H_h(t) = -S^T E_h(t) + \zeta_h^H(t), \\ \varepsilon_\infty \frac{d}{dt} E_h(t) = S H_h(t) - \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} E_h(t) - \sigma E_h(t) + \frac{1}{\tau} P_h(t) + \zeta_h^E(t), \\ \frac{d}{dt} P_h(t) = \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} E_h(t) - \frac{1}{\tau} P_h(t) + \zeta_h^P(t). \end{cases} \quad (8)$$

Next, substituting the exact solutions $E_h(t)$, $H_h(t)$ and $P_h(t)$ into the locally implicit scheme (6) gives the perturbed scheme containing defects (truncation errors) composed of a temporal and a spatial error part. Let δ_k denote the defects for the stages $k = 1, 2, 3$ and 4, we then have the following perturbed scheme

$$\begin{cases} \mu \frac{H_h(t_{n+1/2}) - H_h(t_n)}{\Delta t} = -\frac{1}{2} S^T E_h(t_n) + \delta_1, \\ \varepsilon_\infty \frac{E_h(t_{n+1}) - E_h(t_n)}{\Delta t} = S_0 H_h(t_{n+1/2}) \\ \quad + \frac{1}{2} S_1 (H_h(t_{n+1}) + H_h(t_n)) \\ \quad - \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E_h(t_{n+1}) + E_h(t_n)) \\ \quad - \frac{1}{2} \sigma (E_h(t_{n+1}) + E_h(t_n)) \\ \quad + \frac{1}{2\tau} (P_h(t_{n+1}) + P_h(t_n)) + \delta_2, \\ \frac{P_h(t_{n+1}) - P_h(t_n)}{\Delta t} = \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E_h(t_{n+1}) + E_h(t_n)) \\ \quad - \frac{1}{2\tau} (P_h(t_{n+1}) + P_h(t_n)) + \delta_3, \\ \mu \frac{H_h(t_{n+1}) - H_h(t_{n+1/2})}{\Delta t} = -\frac{1}{2} S^T E_h(t_{n+1}) + \delta_4. \end{cases} \quad (9)$$

Here we multiplied the first equation of (8) for the first and last stages by 1/2 to obtain

$$-\frac{1}{2} S^T E_h(t_n) = \frac{\mu}{2} H'_h(t_n) - \frac{1}{2} \zeta_h^H(t_n),$$

and

$$-\frac{1}{2} S^T E_h(t_{n+1}) = \frac{\mu}{2} H'_h(t_{n+1}) - \frac{1}{2} \zeta_h^H(t_{n+1}).$$

Taking the average of the second relation in (8) written for t_n and for t_{n+1} , we obtain

$$\begin{aligned}
& -\frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E_h(t_{n+1}) + E_h(t_n)) - \frac{1}{2}\sigma(E_h(t_{n+1}) + E_h(t_n)) \\
& + \frac{1}{2\tau} (P_h(t_{n+1}) + P_h(t_n)) \\
= & \frac{1}{2}\varepsilon_\infty (E'_h(t_{n+1}) + E'_h(t_n)) - \frac{1}{2}S(H_h(t_{n+1}) + H_h(t_n)) \\
& - \frac{1}{2}(\zeta_h^E(t_{n+1}) + \zeta_h^E(t_n)),
\end{aligned}$$

and, similarly, from the third equation in (8) we derive

$$\begin{aligned}
& \frac{(\varepsilon_s - \varepsilon_\infty)}{2\tau} (E_h(t_{n+1}) + E_h(t_n)) - \frac{1}{2\tau} (P_h(t_{n+1}) + P_h(t_n)) \\
= & \frac{1}{2} (P'_h(t_{n+1}) + P'_h(t_n)) - \frac{1}{2} (\zeta_h^P(t_{n+1}) + \zeta_h^P(t_n)).
\end{aligned}$$

Inserting the previous expressions into the perturbed scheme (9) yields the defect expressions

$$\begin{aligned}
\delta_1 &= \mu \frac{H_h(t_{n+1/2}) - H_h(t_n)}{\Delta t} - \frac{\mu}{2} H'_h(t_n) + \frac{1}{2} \zeta_h^H(t_n), \\
\delta_2 &= \varepsilon_\infty \frac{E_h(t_{n+1}) - E_h(t_n)}{\Delta t} - \frac{\varepsilon_\infty}{2} (E'_h(t_{n+1}) + E'_h(t_n)) \\
& \quad - S_0 \left[H_h(t_{n+1/2}) - \frac{1}{2} (H_h(t_{n+1}) + H_h(t_n)) \right] \\
& \quad + \frac{1}{2} (\zeta_h^E(t_{n+1}) + \zeta_h^E(t_n)), \\
\delta_3 &= \frac{P_h(t_{n+1}) - P_h(t_n)}{\Delta t} - \frac{1}{2} (P'_h(t_{n+1}) + P'_h(t_n)) \\
& \quad + \frac{1}{2} (\zeta_h^P(t_{n+1}) + \zeta_h^P(t_n)), \\
\delta_4 &= \mu \frac{H_h(t_{n+1}) - H_h(t_{n+1/2})}{\Delta t} - \frac{\mu}{2} H'_h(t_{n+1}) + \frac{1}{2} \zeta_h^H(t_{n+1}).
\end{aligned} \tag{10}$$

Herein we can distinguish the temporal error parts and the spatial error parts contained in the ζ_h^E , ζ_h^H and ζ_h^P contributions. Our interest lies in the temporal errors. We therefore simplify our derivations by omitting these spatial contributions. Carrying the spatial contributions along in the derivations just complicates the formulas and will not lead to different conclusions for

the temporal errors. Finally, the formal Taylor expansion at $t_{n+1/2}$ delivers the temporal defect expressions

$$\begin{aligned}
\delta_1 &= \mu \sum_{k=2} \left(\frac{1}{(k-1)!} - \frac{1}{k!} \right) \frac{(-1)^k}{2^k} (\Delta t)^{k-1} H_h^{(k)}, \\
\delta_2 &= \varepsilon_\infty \sum_{k=2'} \frac{-k}{2^k (k+1)!} (\Delta t)^k E_h^{(k+1)} + S_0 \sum_{k=2'} \frac{1}{2^k k!} (\Delta t)^k H_h^{(k)} \\
&= \delta_5 + S_0 \delta_6, \\
\delta_3 &= \sum_{k=2'} \frac{-k}{2^k (k+1)!} (\Delta t)^k P_h^{(k+1)}, \\
\delta_4 &= \mu \sum_{k=2} \left(\frac{1}{k!} - \frac{1}{(k-1)!} \right) \frac{1}{2^k} (\Delta t)^{k-1} H_h^{(k)},
\end{aligned} \tag{11}$$

where $k = 2'$ means even values for k only, and $E_h^{(k)}$, $H_h^{(k)}$ and $P_h^{(k)}$ the k -th derivatives of $E_h(t)$, $H_h(t)$ and $P_h(t)$ at $t = t_{n+1/2}$. Note that the expansions for δ_1 and δ_4 start with Δt and the expansions for δ_3 , δ_5 and δ_6 with Δt^2 .

4.2. The global error recursion

We introduce the global errors $\mathcal{E}_n^E = E_h(t_n) - E^n$, $\mathcal{E}_n^H = H_h(t_n) - H^n$ and $\mathcal{E}_n^P = P_h(t_n) - P^n$ and the intermediate global error $\mathcal{E}_{n+1/2}^H = H_h(t_{n+1/2}) - H^{n+1/2}$. Subtracting (9) from (6) gives the global errors

$$\begin{aligned}
\mathcal{E}_{n+1/2}^H &= \mathcal{E}_n^H - \frac{\Delta t}{2\mu} S^T \mathcal{E}_n^E + \frac{\Delta t}{\mu} \delta_1, \\
\mathcal{E}_{n+1}^E &= \mathcal{E}_n^E + \frac{\Delta t}{\varepsilon_\infty} S_0 \mathcal{E}_{n+1/2}^H + \frac{\Delta t}{2\varepsilon_\infty} S_1 (\mathcal{E}_{n+1}^H + \mathcal{E}_n^H) \\
&\quad - \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\varepsilon_\infty \tau} (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) \\
&\quad - \frac{\Delta t}{2\varepsilon_\infty} \sigma (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) + \frac{\Delta t}{2\varepsilon_\infty \tau} (\mathcal{E}_{n+1}^P + \mathcal{E}_n^P) + \frac{\Delta t}{\varepsilon_\infty} \delta_2, \\
\mathcal{E}_{n+1}^P &= \mathcal{E}_n^P + \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\tau} (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) - \frac{\Delta t}{2\tau} (\mathcal{E}_{n+1}^P + \mathcal{E}_n^P) \\
&\quad + \Delta t \delta_3, \\
\mathcal{E}_{n+1}^H &= \mathcal{E}_{n+1/2}^H - \frac{\Delta t}{2\mu} S^T \mathcal{E}_{n+1}^E + \frac{\Delta t}{\mu} \delta_4.
\end{aligned} \tag{12}$$

From the first and fourth equations of (12) we get

$$\begin{aligned}\mathcal{E}_{n+1/2}^H &= \mathcal{E}_n^H - \frac{\Delta t}{2\mu} S^T \mathcal{E}_n^E + \frac{\Delta t}{\mu} \delta_1, \\ \mathcal{E}_{n+1/2}^H &= \mathcal{E}_{n+1}^H + \frac{\Delta t}{2\mu} S^T \mathcal{E}_{n+1}^E - \frac{\Delta t}{\mu} \delta_4.\end{aligned}\tag{13}$$

Eliminating the intermediate error in the second equation of the global error scheme by inserting half of each expression of (13) yields

$$\begin{aligned}\mathcal{E}_{n+1}^E - \mathcal{E}_n^E &= \frac{\Delta t}{\varepsilon_\infty} S_0 \left[\frac{1}{2} (\mathcal{E}_{n+1}^H + \mathcal{E}_n^H) + \frac{\Delta t}{2\mu} \left(S^T \frac{(\mathcal{E}_{n+1}^E - \mathcal{E}_n^E)}{2} + (\delta_1 - \delta_4) \right) \right] \\ &\quad + \frac{\Delta t}{2\varepsilon_\infty} S_1 (\mathcal{E}_{n+1}^H + \mathcal{E}_n^H) - \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\varepsilon_\infty \tau} (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) \\ &\quad - \frac{\Delta t}{2\varepsilon_\infty} \sigma (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) + \frac{\Delta t}{2\varepsilon_\infty \tau} (\mathcal{E}_{n+1}^P + \mathcal{E}_n^P) + \frac{\Delta t}{\varepsilon_\infty} \delta_2, \\ &= - \left(\frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\varepsilon_\infty \tau} + \frac{\Delta t}{2\varepsilon_\infty} \sigma \right) (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) \\ &\quad + \frac{\Delta t^2}{4\varepsilon_\infty \mu} S_0 S^T (\mathcal{E}_{n+1}^E - \mathcal{E}_n^E) + \frac{\Delta t}{2\varepsilon_\infty} S (\mathcal{E}_{n+1}^H + \mathcal{E}_n^H) \\ &\quad + \frac{\Delta t}{2\varepsilon_\infty \tau} (\mathcal{E}_{n+1}^P + \mathcal{E}_n^P) + \frac{\Delta t}{\varepsilon_\infty} \left(\delta_2 + \frac{\Delta t}{2\mu} S_0 (\delta_1 - \delta_4) \right).\end{aligned}$$

We eliminate the intermediate error in the fourth equation in (12) by using the first expression of (13) to obtain the following global error schemes :

$$\begin{aligned}\mathcal{E}_{n+1}^E &= \mathcal{E}_n^E - \left(\frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\varepsilon_\infty \tau} + \frac{\Delta t}{2\varepsilon_\infty} \sigma \right) (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) \\ &\quad + \frac{\Delta t^2}{4\varepsilon_\infty \mu} S_0 S^T (\mathcal{E}_{n+1}^E - \mathcal{E}_n^E) \\ &\quad + \frac{\Delta t}{2\varepsilon_\infty} S (\mathcal{E}_{n+1}^H + \mathcal{E}_n^H) + \frac{\Delta t}{2\varepsilon_\infty \tau} (\mathcal{E}_{n+1}^P + \mathcal{E}_n^P) + \Delta t \delta_n^E, \\ \mathcal{E}_{n+1}^P &= \mathcal{E}_n^P - \frac{\Delta t}{2\tau} (\mathcal{E}_{n+1}^P + \mathcal{E}_n^P) + \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\tau} (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) + \Delta t \delta_n^P, \\ \mathcal{E}_{n+1}^H &= \mathcal{E}_n^H - \frac{\Delta t}{2\mu} S^T (\mathcal{E}_{n+1}^E + \mathcal{E}_n^E) + \Delta t \delta_n^H,\end{aligned}\tag{14}$$

where

$$\begin{aligned}
\delta_n^E &= \frac{1}{\varepsilon_\infty} \left(\delta_2 + \frac{\Delta t}{2\mu} S_0 (\delta_1 - \delta_4) \right) \\
&= \frac{1}{\varepsilon_\infty} \left(\delta_5 + S_0 \left(\frac{\Delta t}{2\mu} (\delta_1 - \delta_4) + \delta_6 \right) \right), \\
\delta_n^P &= \delta_3, \\
\delta_n^H &= \frac{1}{\mu} (\delta_1 + \delta_4).
\end{aligned} \tag{15}$$

From the expressions of δ_k with $k = 1, 2, 3, 4, 5$ in (11) we observe that these three new defects contain only even terms in Δt and start with Δt^2 . At this stage we assume that $E_h(t)$, $H_h(t)$ and $P_h(t)$ belong to $C^3[0, T]$. It follows from the remainder in Taylor's theorem that for $\Delta t \sim h$, $h \rightarrow 0$,

$$\delta_5 = \mathcal{O}(\Delta t^2), \quad \frac{\Delta t}{2\mu} (\delta_1 - \delta_4) + \delta_6 = \mathcal{O}(\Delta t^2), \quad \delta_n^P = \mathcal{O}(\Delta t^2), \quad \delta_n^H = \mathcal{O}(\Delta t^2). \tag{16}$$

Let

$$\mathcal{E}_n = \begin{pmatrix} \mathcal{E}_n^H \\ \mathcal{E}_n^P \\ \mathcal{E}_n^E \end{pmatrix}, \quad \delta_n = \begin{pmatrix} \delta_n^H \\ \delta_n^P \\ \delta_n^E \end{pmatrix},$$

and

$$\varepsilon_1 = 1 + \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\varepsilon_\infty \tau} + \frac{\Delta t}{2\varepsilon_\infty} \sigma, \quad \varepsilon_2 = 1 - \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\varepsilon_\infty \tau} - \frac{\Delta t}{2\varepsilon_\infty} \sigma.$$

From (14) we can write the global error in a more compact form (one-step recurrence relation)

$$\mathcal{E}_{n+1} = R\mathcal{E}_n + \Delta t \rho_n, \quad R = R_L^{-1} R_R, \quad \rho_n = R_L^{-1} \delta_n, \tag{17}$$

where

$$R_L = \begin{pmatrix} I & 0 & \frac{\Delta t}{2\mu} S^T \\ 0 & \left(1 + \frac{\Delta t}{2\tau}\right) I & -\frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\tau} I \\ -\frac{\Delta t}{2\varepsilon_\infty} S & -\frac{\Delta t}{2\varepsilon_\infty \tau} I & \varepsilon_1 I - \frac{\Delta t^2}{4\varepsilon_\infty \mu} S_0 S^T \end{pmatrix},$$

$$R_R = \begin{pmatrix} I & 0 & -\frac{\Delta t}{2\mu} S^T \\ 0 & \left(1 - \frac{\Delta t}{2\tau}\right) I & \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\tau} I \\ \frac{\Delta t}{2\varepsilon_\infty} S & \frac{\Delta t}{2\varepsilon_\infty \tau} I & \varepsilon_2 I - \frac{\Delta t^2}{4\varepsilon_\infty \mu} S_0 S^T \end{pmatrix},$$

and \mathcal{E}_n , $\Delta t \rho_n$ and δ_n are respectively the (space-time) global, local and truncation errors. The recursion (17) has the standard form featured in the convergence analysis of one-step integration methods, see e.g. [17]. Assuming Lax-Richtmyer stability, whereby we assume R_L inversely bounded for $\Delta t \sim h$, $h \rightarrow 0$, it transfers local errors to the global error by essentially adding all local errors. It reveals second order ODE convergence for a fixed spatial dimension since then S_0 within the defect δ_n^E is bounded and hence $\rho_n = \mathcal{O}(\Delta t^2)$ for $\Delta t \rightarrow 0$, because (15) and (16) yield that δ_n^E , δ_n^P and δ_n^H are $\mathcal{O}(\Delta t^2)$. However, for a simultaneous space-time grid refinement, the local error component δ_n^E must have components which will grow with h^{-1} . This growth is unavoidable, since by definition of $S_1 = SS_H$ we have

$$S_0 = S - S_1 = S(I - S_H), \quad (18)$$

and $S = \mathcal{O}(h^{-1})$. Therefore we have $\delta_n^E = \mathcal{O}(\Delta t)$ for $\Delta t \sim h$, $h \rightarrow 0$. The local errors δ_n^P and δ_n^H cause no problem as they contain only solution derivatives, thus δ_n^P and δ_n^H are $\mathcal{O}(\Delta t^2)$, for $\Delta t \sim h$, $h \rightarrow 0$.

Fortunately, this order reduction by one order of Δt manifests itself only in the local error and cancels in the transition from the local to the global error. This cancellation can be proven by transforming the global error scheme (17) into one where local errors remain second-order for $\Delta t \sim h$, $h \rightarrow 0$.

4.3. A transformed global error recursion

The transformation emanates from [17], Lemma II.2.3. and reveals that the second-order will be maintained for any stable space-time grid refinement $\Delta t \sim h$, $h \rightarrow 0$. From this lemma we can assume that if the local error $\Delta t \rho_n$ allows a decomposition

$$\Delta t \rho_n = (I - R) \xi_n + \eta_n, \quad (19)$$

such that $\xi_n = \mathcal{O}(\Delta t^2)$ and $\eta_n = \mathcal{O}(\Delta t^3)$, for $\Delta t \sim h$, $h \rightarrow 0$, then we have the desired second order convergence for \mathcal{E}_n . Therefore, it remains to

check (19), which amounts to examining $\Delta t \rho_n = \Delta t R_L^{-1} \delta_n = (I - R) \xi_n + \eta_n = (I - R_L^{-1} R_R) \xi_n + \eta_n$, or equivalently,

$$\Delta t R_L^{-1} \begin{pmatrix} \delta_n^H \\ \delta_n^P \\ \delta_n^E \end{pmatrix} = R_L^{-1} (R_L - R_R) \begin{pmatrix} \xi_n^H \\ \xi_n^P \\ \xi_n^E \end{pmatrix} + R_L^{-1} R_L \begin{pmatrix} \eta_n^H \\ \eta_n^P \\ \eta_n^E \end{pmatrix},$$

which yields

$$\begin{pmatrix} \Delta t \delta_n^H \\ \Delta t \delta_n^P \\ \Delta t \delta_n^E \end{pmatrix} = (R_L - R_R) \begin{pmatrix} \xi_n^H \\ \xi_n^P \\ \xi_n^E \end{pmatrix} + R_L \begin{pmatrix} \eta_n^H \\ \eta_n^P \\ \eta_n^E \end{pmatrix},$$

or

$$\begin{aligned} \Delta t \delta_n^H &= \frac{\Delta t}{\mu} S^T \xi_n^E + \eta_n^H + \frac{\Delta t}{2\mu} S^T \eta_n^E, \\ \Delta t \delta_n^P &= \frac{\Delta t}{\tau} \xi_n^P - \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{\tau} \xi_n^E + \left(1 + \frac{\Delta t}{2\tau}\right) \eta_n^P - \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\tau} \eta_n^E, \\ \Delta t \delta_n^E &= -\frac{\Delta t}{\varepsilon_\infty} S \xi_n^H - \frac{\Delta t}{\varepsilon_\infty \tau} \xi_n^P + \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{\varepsilon_\infty \tau} \xi_n^E + \frac{\Delta t}{\varepsilon_\infty} \sigma \xi_n^E \\ &\quad - \frac{\Delta t}{2\varepsilon_\infty} S \eta_n^H - \frac{\Delta t}{2\varepsilon_\infty \tau} \eta_n^P + \eta_n^E + \frac{(\varepsilon_s - \varepsilon_\infty) \Delta t}{2\varepsilon_\infty \tau} \eta_n^E \\ &\quad + \frac{\Delta t}{2\varepsilon_\infty} \sigma \eta_n^E - \frac{\Delta t^2}{4\varepsilon_\infty \mu} S_0 S^T \eta_n^E. \end{aligned} \tag{20}$$

Thus, our task is now to identify error vectors $\xi_n^E, \xi_n^H, \xi_n^P$ and $\eta_n^E, \eta_n^H, \eta_n^P$ in accordance with (19) such that (20) are satisfied. Let us first define

$$\eta_n^H = \frac{\Delta t}{\mu} (\delta_1 + \delta_4), \eta_n^P = \Delta t \delta_3 \text{ and } \eta_n^E = \frac{\Delta t}{\varepsilon_\infty} \delta_5. \tag{21}$$

From (16), we observe that η_n^H, η_n^P and η_n^E behave like $\mathcal{O}(\Delta t^3)$. Next from (20) we identify error vectors $\xi_n^E, \xi_n^H, \xi_n^P$. From the first equation of (20) and the definition of δ_n^H (see (15)) we write

$$\frac{\Delta t}{\mu} (\delta_1 + \delta_4) = \frac{\Delta t}{\mu} S^T \xi_n^E + \eta_n^H + \frac{\Delta t}{2\mu} S^T \eta_n^E. \tag{22}$$

Substituting $(\Delta t/\mu)(\delta_1 + \delta_4) = \eta_n^H$ into (22) reveals the error vector ξ_n^E

$$\xi_n^E = -\frac{1}{2}\eta_n^E \quad \left(= -\frac{\Delta t}{2\varepsilon_\infty}\delta_5 \right),$$

hence $\xi_n^E = \mathcal{O}(\Delta t^3)$. Furthermore

$$\xi_n^P = -\frac{1}{2}\eta_n^P \quad \left(= -\frac{\Delta t}{2}\delta_3 \right),$$

hence $\xi_n^P = \mathcal{O}(\Delta t^3)$. Thus, it remains to identify ξ_n^H and to check if $\xi_n^H = \mathcal{O}(\Delta t^2)$. Simple calculations show that

$$S\xi_n^H = -\frac{1}{2}S\eta_n^H - \frac{\Delta t}{4\mu}S_0S^T\eta_n^E - S_0\left(\frac{\Delta t}{2\mu}(\delta_1 - \delta_4) + \delta_6\right), \quad (23)$$

and using $S_0 = S(I - S_H)$ this clearly shows that $\xi_n^H = \mathcal{O}(\Delta t^2)$. Consequently, we have proven that the subdivision into coarse and fine elements is not detrimental to the second order ODE convergence of the method (6), under stable simultaneous space-time grid refinement towards the exact underlying PDE solution. We summarize this convergence result with the following theorem.

Theorem 1. *Let $H_h(t)$, $E_h(t)$ and $P_h(t)$ denote the exact solutions of the Maxwell problem in dispersive media under consideration, restricted to the space grid, i.e. the exact solutions of the system of ODEs*

$$\begin{cases} \mu \frac{d}{dt} H_h(t) = -S^T E_h(t) + \zeta_h^H(t), \\ \varepsilon_\infty \frac{d}{dt} E_h(t) = S H_h(t) - \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} E_h(t) - \sigma E_h(t) + \frac{1}{\tau} P_h(t) + \zeta_h^E(t), \\ \frac{d}{dt} P_h(t) = \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} E_h(t) - \frac{1}{\tau} P_h(t) + \zeta_h^P(t), \end{cases} \quad (24)$$

where ζ_h^H , ζ_h^E and ζ_h^P denote the spatial truncation errors. Assume a Lax-Richtmyer stable space-time grid refinement $\Delta t \sim h$, $h \rightarrow 0$. On the interval $[0, T]$ the approximations H^n , E^n and P^n of method (6) then converge with order two to $H_h(t)$, $E_h(t)$ and $P_h(t)$.

5. Numerical simulations : microwave propagation in head tissues

The order of convergence of the method obtained in the previous Theorem has been confirmed by numerical simulations in [15] with artificial three-dimensional problems, and in [18] with artificial two-dimensional problems, on the cube $[0, 1]^3$ with an exact solution of the propagation of a standing wave in a cubic PEC cavity. Significant gains of CPU time have also been observed, about 8 times lower than the fully explicit case, showing the efficiency of the method.

We present here numerical results for a realistic problem demonstrating the application of the proposed locally implicit DGTD method (6) to microwave propagation in biological tissues. For that purpose, we consider an heterogeneous geometrical model of the head consisting of four tissues namely, the skin, the skull, the Cerebro Spinal Fluid (CSF) and the brain. The surface meshes of the different tissues are shown on Figure 1. The computational domain is artificially bounded by a sphere on which a Silver-Müller condition is imposed and we use a relatively coarse unstructured tetrahedral mesh consisting of 61,358 vertices and 366,208 tetrahedra, the implicit treatment corresponding to 5092 tetrahedra, so approximately 1.4% of the mesh. This mesh is shown on Figure 2. The Debye model parameters that we have used for the tissues are given in the Table 1.

Tissue	Skin	Skull	CSF	Brain
ε_∞	1.0	1.0	2.0	1.0
$\varepsilon_s - \varepsilon_\infty$	38.0	10.5	66.0	43.0
τ (ps)	10.0	20.0	10.0	10.0
σ (S·m ⁻¹)	0.7	0.1	2.0	0.7

Table 1: Debye model parameters for the different tissues.

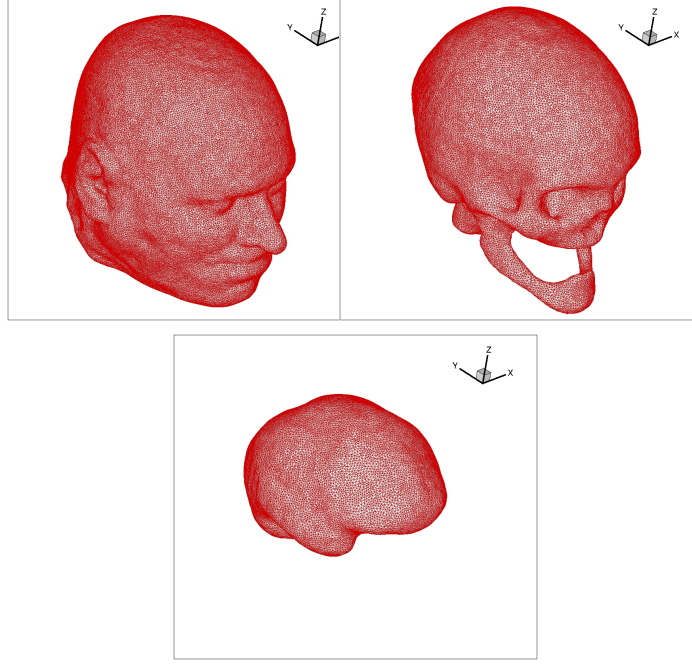


Figure 1: Surface meshes of the skin, the skull and the CSF

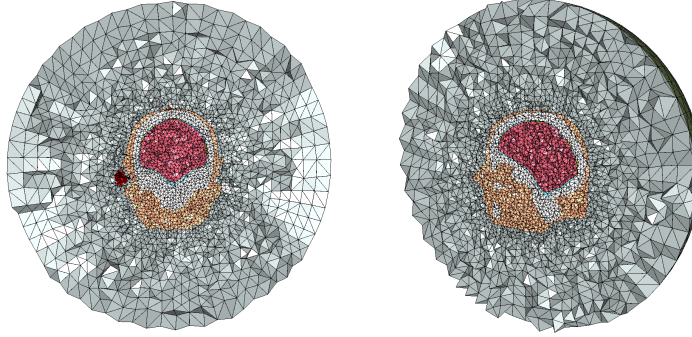


Figure 2: Cross sections of the 3D mesh (61,358 vertices, 366,208 tetrahedra, implicit treatment: 5092 tetrahedra, 1.4% of the mesh, *dark red region*).

The incident field is a plane wave propagating in the z direction, with a temporal evolution given by a modulated Gaussian pulse,

$$s(t) = e^{-\left(\frac{t-4t_p}{t_p}\right)^2} \sin(2\pi f_c(t - t_p)). \quad (25)$$

We perform a simulation with the locally implicit DGTD- \mathbb{P}_1 method

with a centered flux and a space discretization of order 1) using the above-mentioned incident field. The total simulation time is equal to 9 h 57 min. Time evolution of the electric component E^z is shown on Figure 3.

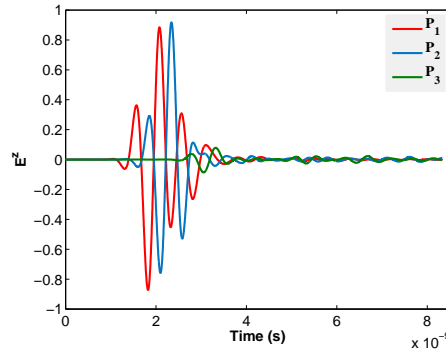


Figure 3: Microwave propagation in head tissues: time evolution of the E^z component of the electric field at selected spatial locations, $\vec{P}_1 = (-0.1962, -0.0027, -0.0032)$, $\vec{P}_2 = (-0.1013, -0.0009, 0.0000)$ and $\vec{P}_3 = (0.0985, -0.0019, -0.0004)$.

On Figure 4 we show the contour lines of the local SAR (Specific Absorption Rate) normalized by the maximal local SAR, in logarithmic scale, for the calculations with the locally implicit DGTD- \mathbb{P}_1 method (6). We recall that the SAR is a measure of the rate at which electric energy is absorbed by the tissues when exposed to a radio-frequency electromagnetic field. It represents the power absorbed per mass of tissue and has units of watts per kilogram ($\text{W} \cdot \text{kg}^{-1}$). The SAR is then defined as $\sigma |\vec{E}_{Four}|^2 / \rho$, where \vec{E}_{Four} denotes the electric field in the frequency-domain, resulting from the discrete Fourier transform of the temporal field, and ρ is the density which depends on the tissues.

6. Conclusion

In this work we have conducted a study of a locally implicit discontinuous Galerkin time domain method for electromagnetic wave propagation in dispersive media. We have shown the stability of the method and derive a convergence analysis to prove that the method retains its second order convergence. Numerical simulations in 3D show the efficiency of this method. Following the techniques developed in the recent preprint [19] we think that it is also possible to give a bound of the error between the exact solution and the DG discretization.

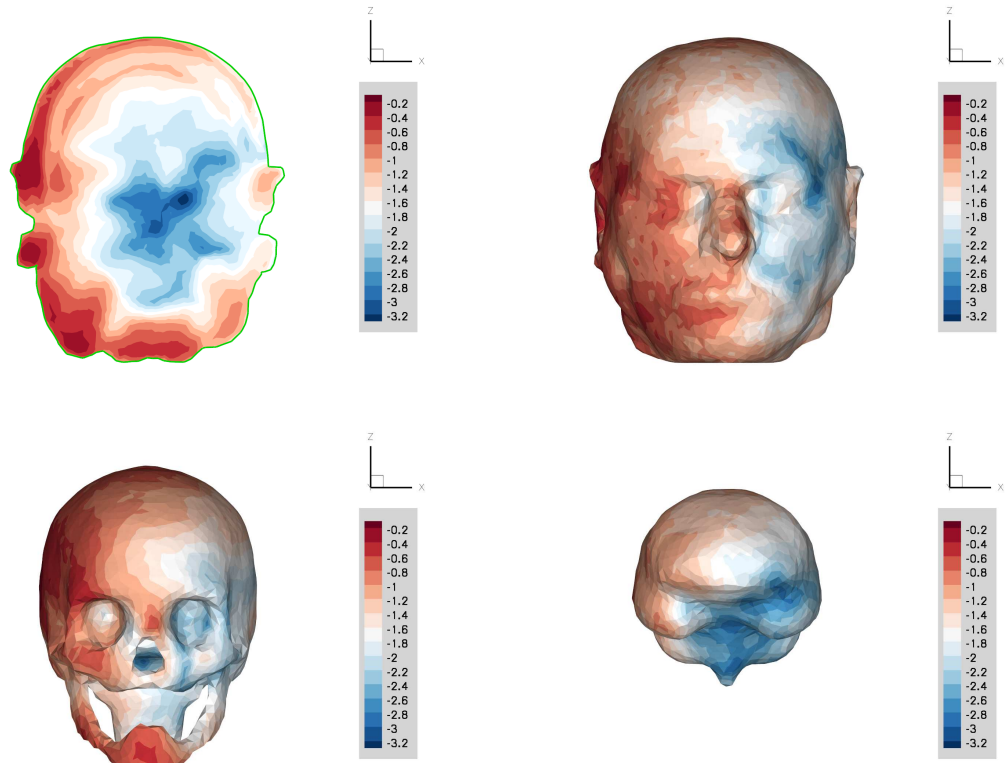


Figure 4: Microwave propagation in head tissues: calculation using a pulse in time plane wave as the incident field. Contour lines of the local SAR normalized by the maximal local SAR (logarithmic scale).

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